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Anomalous behaviour of Zr-Cu metallic glass superconductors

A K Mondal, B Banerjee and S K Roy*
Department of Physics, Visva-Bharati University, Santiniketan-731 235, West Bengal, India

E-mail : roysamar@rediffmail.com

Abstract : The studies on the properties of binary – metallic glass alloys particularly those based on Zr have been made An increase in the resistance is reported near the superconducting transition temperature for metallic alloys which is an anomalous behaviour for such alloys This anomaly consists of a peak in the resistance which can reach upto 10 μW-cm above the usual superconducting fluctuation region Although, many such anomalous properties have been accounted for weak localization and interacting contributions, the question of origin of these effects are still highly controversial and not yet properly understood We analyse the probable effects that can cause the fluctuation of superconducting transition temperature (T_c) We try to reinvestigate the fluctuation of superconducting transition temperature (T_c) through the deduction of superconducting gap parameter and the resistivity behavior from the evaluation of the normal state electronic property for some Zr-Cu alloys The results have been attributed to the weak localisation and *s-d* exchange interactions due to the presence of localised electrons on the Cu sites

Keywords Resistivity peaks, transition temperature, *s-d* exchange interaction

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1. Introduction

The Zr-Cu binary metallic superconducting alloys have been found to be of immense experimental and theoretical interest as many anomalous behaviors are reported for these samples. One such very important anomaly is the resistance close to the superconducting transition temperature. We refer to such anomalies observed [1, 2] in superconducting transition temperature of Zr_{60}- Cu_{40} and Zr_{50}–Cu_{50} alloys. This anomaly consists of a peak in the resistance which can reach upto 10μΩcm above the usual superconducting fluctuation region. Many [3,4] of such anomalous properties have been attributed to weak localization and interaction contributions. But the question of origin of these effects are still highly controversial and not yet properly understood.

The purpose of this paper is therefore, to analyse the probable effects and explain the behavior of anomalous resistivity near the superconducting transition temperature for some Zr-Cu alloys. We attempt to look into this fluctuation through the deduction of resistivity behavior from the normal state electronic properties. We conjecture that the anomalous resistivity behavior is due to the *s-d* exchange interaction between the conduction electrons and localized moments however small it may be.

*Corresponding Author

Due to the presence of Cu, a small *s–d* exchange interaction between the conduction electrons and those localized on the Cu sites may result in the increase in resistivity near the onset of superconducting transition temperature.

2. Formulation of the Hamiltonian

We write a Hamiltonian for Zr-Cu system which modifies the BCS Hamiltonian due to the presence of *s-d* exchange interaction term.

The Hamiltonian for such a system may be written as

$$H = \sum_{k\sigma} \varepsilon_k c^{\dagger}_{k\sigma} c_{k\sigma} - V \sum_{kk'} c^{\dagger}_{k'\uparrow} c^{\dagger}_{-k\downarrow} c_{-k\downarrow} c'_{k\uparrow}$$

$$-\frac{J}{2N} \sum_{kk'} \left[\left(c^{\dagger}_{k\uparrow} c_{k'\uparrow} - c^{\dagger}_{k\downarrow} c_{k'\uparrow} \right) S_z + c^{\dagger}_{k\uparrow} c_{k'\downarrow} S_- \right.$$

$$\left. + c^{\dagger}_{k\downarrow} c_{k'\uparrow} S_+ \right] , \quad (1)$$

where the first term represents the single particle energy; the second term the BCS Hamiltonian with usual pairing interaction V and the last term represents the *s-d* interaction term between the conduction electrons and the localized moments at the impurity sites. N is the total number of atoms in the system, J

the strength of the s-d interaction. S_+ and S_- are the components of the spin operator and $c^{\dagger}_{k\sigma}, c_{k\sigma}$ are the usual creation and annihilation operators of the conduction electrons with wavevector k and spin σ.

The Hamiltonian (1) after mean field approximation may be written as

$$H_{MF} = \sum_{k\sigma} \varepsilon_k c^{\dagger}_{k\sigma} c_{k\sigma} - \Delta \sum \left(c^{\dagger}_{k\uparrow} c^{\dagger}_{-k\downarrow} + c_{k\uparrow} c_{-k\downarrow} \right)$$

$$- \frac{3J}{2N} \sum_{kk'\sigma} \left(n_{k'} - \frac{1}{2} \right) c^{\dagger}_{k\sigma} c_{k'\sigma}, \tag{2}$$

where n_k is the fermion occupation number and Δ the superconducting order parameter defined by

$$\Delta = \sum V \left\langle c^{\dagger}_{k\uparrow} c^{\dagger}_{-k\downarrow} \right\rangle = \sum \left\langle c_{k\uparrow} c_{-k\downarrow} \right\rangle. \tag{3}$$

3. Methodology

Eq. (2) is now solved for the gap parameter and the normal state resistivities by defining the temperature dependent Green's functions

$$G^{(1)}_{pq}(t) = \left\langle\left\langle c_{p\uparrow}(t), c^{\dagger}_{q\uparrow}(0) \right\rangle\right\rangle \tag{4}$$

$$G^{(2)}_{pq}(t) = \left\langle\left\langle c^{\dagger}_{-p\downarrow}(t); c^{\dagger}_{q\uparrow}(0) \right\rangle\right\rangle. \tag{5}$$

The Green's functions given by eq. (4) and equation (5) are solved by equation of motion method involving the Hamiltonian eq. (2) and taking the Fourier transform. We thus obtain the normal state and the gap Green's function in the coupled form as

$$(E - \varepsilon_p) G^{(1)}_{pq}(E) = \delta_{pq} - \Delta G^{(2)}_{pq}(E)$$

$$\frac{3J}{2N} \sum_{kk'} \left(n_{k'} - \frac{1}{2} \right) G^{(1)}_{k'q}(E), \tag{6}$$

$$(E + \varepsilon_p) G^{(2)}_{pq}(E) = -\Delta G^{(1)}_{pq}(E)$$

$$\frac{}{2N} \sum_{kk'} \left(n_{k'} - \frac{1}{2} \right) G^{(2)}_{k'q}(E). \tag{7}$$

These equations are decoupled retaining only the linear term in J as J has been assumed to be very weak for single impurity case. We thus finally obtain

$$G^{(1)}_{pp}(E) = \frac{}{E - \varepsilon_n} \quad 1 - \frac{\sum_p \frac{3J}{2N}\left(n_p - \frac{}{2}\right.}{(E - \varepsilon_n)\left(1 + \frac{\frac{3J}{2N}\sum_p \left(n_p - \frac{1}{2}\right)}{(E - \varepsilon_p)}\right.} \tag{8}$$

$$G^{(1)}_{pp}(E) = -\frac{\Delta}{\left(E^2 - \varepsilon_p^2\right)} \quad 1 - \frac{\frac{3J}{2N}\sum_p \left(n_p - \frac{1}{2}\right)}{(E - \varepsilon_n)} \tag{9}$$

We now define the function

$$G^{(0)}(E) = \frac{1}{N} \sum_{k'} \frac{\left(n_{k'} - \frac{1}{2}\right)}{(E - \varepsilon_{k'})} = K(E) - iL(E), \tag{10}$$

where $K(E)$ and $L(E)$ are real functions of E and are defined by

$$K(E) = \frac{1}{N} \sum_{k'} \frac{P\left(n_{k'} - \frac{1}{2}\right)}{E - \varepsilon_{k'}}$$

and

$$L(E) = \rho\pi \left[n_{k'} - \frac{1}{2} \right],$$

where ρ denotes the Fermi surface density of states of conduction electrons. In eq. (11), we replace the sum over $K(E)$ by the integral over $\varepsilon_{k'}$. Now, if we assume the density of states to be independent of $\varepsilon_{k'}$ at the Fermi surface, the integrand diverges. Thus, we should cut-off the integration from $(-D)$ to (D)

$$K(E) = \frac{\rho}{2N} \int_{-D}^{D} P\left(\frac{1}{E - \varepsilon_{k'}} \right) \tanh\left(\frac{\varepsilon_{k'}}{2T} \right) d\varepsilon_{k'}. \tag{13}$$

4. Resistivity calculations from normal and anomalous Green's function

The resistivity of Zr-Cu alloys have been calculated from the imaginary part of the normal state Green's function. The s-d exchange strength term J is obtained from the gap parameter Green's function eq. (9). The alloy gap function may be obtained from the usual gap equation

$$\Delta = -\frac{1}{\beta} \sum_p V . G^{(2)}_{pp}(E) \tag{14}$$

This is obtained as

$$1 + \frac{3}{2} JK(\varepsilon_p) = V \int_{T}^{T_c} \rho(\varepsilon_p) . \frac{1}{\varepsilon_p} \tanh\left(\frac{\varepsilon_p}{2T} \right) d\varepsilon_p \tag{15}$$

$$= V_\rho(0) \ln\left(1.02 \, T_c \right. \tag{16}$$

at $T \approx T_c + 0$.

To calculate the resistivity change due to the scattering of conduction electrons from the impurity sites we need to calculate the lifetime τ_k defined by the equation

$$\frac{1}{\tau_k} = \mathrm{Im}\left[G_{pp}^{(1)}(E)\right]^{-1}. \tag{17}$$

From the Green's function (8), we have

$$\left[G_{pp}^{(1)}(E)\right]^{-1} = \left(E - \varepsilon_p\right) + \frac{\sum_p \frac{3J\left(n_p - \frac{1}{2}\right)}{2N}}{1 + \frac{3JG(0)}{2}(E)} \tag{18}$$

Using eq. (9), we can split eq. (18) in real and imaginary parts

$$\left[G_{pp}^{(1)}(E)\right]^{-1} = \left(E - \varepsilon_p\right) + \frac{\Gamma X}{\pi(X^2 + \Gamma^2)} + i\frac{\Gamma^2}{\pi(X^2 + \Gamma^2)} \tag{19}$$

where, $X = 1 + \frac{3}{2}JK(E)$ and $\Gamma = \frac{3}{2}JL(E)$.. Thus, the imaginary part of eq. (19) combined with eq. (16) yields

$$\frac{1}{\tau_k} = \frac{\Gamma^2}{\pi\left(X^2 + \Gamma^2\right)}. \tag{20}$$

Now from general transport equation, the conductivity σ can be written as [5]

$$\sigma = -\frac{e^2 n}{m^*}\int_{-\infty}^{\infty} \tau_k \frac{\partial f(\varepsilon_p)}{\partial \varepsilon_p} d\varepsilon_p, \tag{21}$$

where n is the total number of conduction electrons, m^* is the effective mass and $f(\varepsilon_p)$ is the fermi distribution function.

The resistivities R are calculated for $T \approx T_c + 0$, from eqs. (20) and (21). We thus have,

$$\frac{R_T}{R_{T_c}} = \frac{\Gamma^2}{\left[V_p(\varepsilon_p)\ln\left(\frac{D'T_c}{DT}\right)\right]^2 + \pi\Gamma^2}, \tag{22}$$

where $R_0 = \frac{m^*}{e^2 n}$ at $T = T_c$.

The values of $L(\varepsilon_p)$ has been calculated from the Fermi function near Fermi surface given by

$$L(\varepsilon_p) = \pi\rho(\varepsilon_p)\left[\frac{1}{1 + \exp\left(\frac{\varepsilon_p}{kT_c}\right)} - \frac{1}{2}\right]$$

$$= \frac{\pi\rho(\varepsilon_p)}{2}\tanh\left(\frac{T}{2T_c}\right). \tag{23}$$

Now at $T = T_c + 0$,

$$L(\varepsilon_p) = \frac{\pi\rho(0)}{2}\tanh\left(\frac{T}{2T_c}\right) \tag{24}$$

Final equations for $\frac{R_T}{R_{T_c}}$ with $T = T_c + 0$, may be written using the electron-phonon coupling constant $\lambda_{ep} = V_p(0)$ at the Fermi surface from [5] and (16) as

$$\frac{R_T}{R_{T_c}} = \frac{3J\pi\tanh\left(\frac{T}{2T_c}\right)}{V\ln\frac{D'T_c}{DT}\;\;\frac{3J\pi\tanh\left(\frac{T}{2T_c}\right)}{4}}^{-2}. \tag{25}$$

5. Results and discussion

The Cooper pairing potential V has been evaluated from the band structure density of states $N_b(0)$ values given in [4] and the λ_{ep} values given in [6]. Following the experimental findings on $Zr_{60} - Cu_{40}$ and Zr_{50}–Cu_{50} samples, we have evaluated the resistivity ratios $R(T) / R(T_c)$ for $(T - T_c) = 20$mK, 40mK and 60mK, with $J = 0.006$ and 0.0001 respectively. The variations of $\frac{R(T)}{R(T_c)}$ have been shown in Figures. 1 and 2. We emphasise that the observation of peaks are the natural consequences of reported theoretical divergence in the resistivity expression with 20-60mK of T_c which are in good qualitative agreement with the experimental results. These results strongly suggest that the

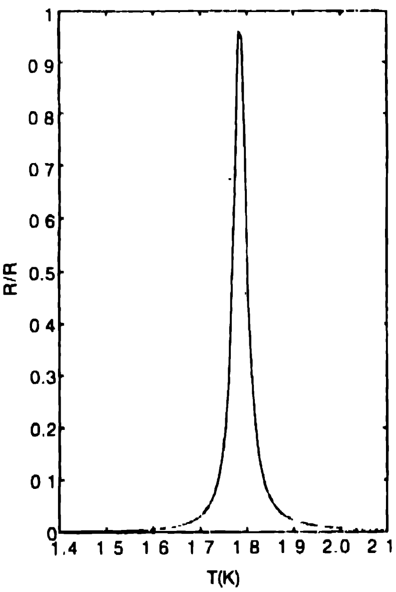

Figure 1. Normalised plot of variation of resistivity ratio with temperature T(K) with J = 0.006 for impure $Cu_{40}Zr_{60}$, with λ_{eff} = 0.642, T_c = 1.75K, N_o = 0.867 and V = 0.7405eV

peak arises from the weak interaction between the superconducting fluctuation and $s-d$ exchange interaction.

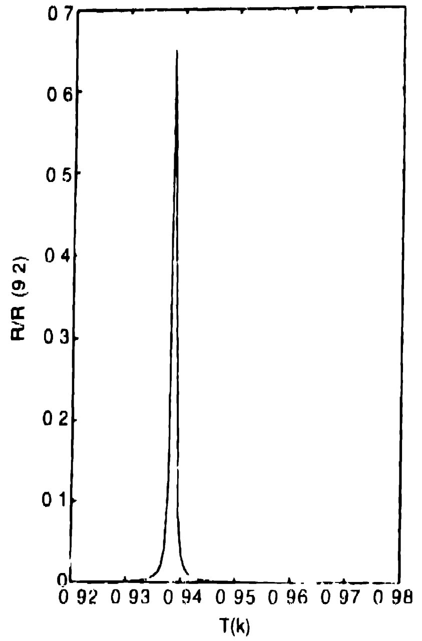

Figure 2. Normalised plot of variation of resistivity ratio with temperature T(K) with J = 0 0001 for impure $Cu_{50}Zr_{50}$ with λ_{eff} = 0 512, T_c = 0 92K, N_o = 0 826 and V = 0 6198547eV

This may be attributed to the weak localization of conduction electrons due to the presence of impurities near the superconducting phase transition.

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